# SOLAR INDUCED CHLOROPHYLL FLUORESCENCE OCO-2 LITE FILES (B7000) USER GUIDE

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#### **Overview Information**

The solar induced fluorescence (SIF) OCO-2 Lite files contain a subset of the information in the IMAP-DOAS (IDP) pre-processing L2 files. There is one file per day, for each day that had at least one retrieved sounding. The main purpose of the SIF-lite files is to a) perform post-processing on the original IDP files and b) provide all valid data in significantly smaller files that still contain all necessary information for typical science analyses. In addition, they have some value added:

- Only contain converged soundings that passed initial quality criteria thresholds
- They include an important SIF correction procedure, performed on a daily basis using non-fluorescing surfaces such as deserts or most oceans
- They contain additional information merged from both the A-band preprocessor (ABP) as well as meteorological input data interpolated to the OCO-2 footprint in time and space

The SIF-lite files are provided in the netCDF-4 format (Unidata hyperlink here). Because netCDF-4 is built on the HDF-5 storage layer, the files may be read with both netCDF4 and HDF5 software, usually available in most computing tools such as Matlab, IDL, python. For python, the use of h5py (http://www.h5py.org/) or netCDF4 (https://github.com/Unidata/netcdf4-python) is recommended and easily available through most python installations on both Linux/Mac and Windows systems.

Generally speaking, each field in the file is described in the Attributes of that field within the file itself. Descriptions for selected fields are given below, but please be sure to read the Attributes of each used field within the actual Lite file. HDFview (Hyperlink) is a good tool to quickly browse individual datasets for their content, attributes and so forth. Figure 1 shows a HDFview screenshot, enabling a quick overview of the general structure of the SIF-lite files. Ancillary information from the OCO-2 cloud pre-processors (IMAP-DOAS IDP and Oxygen A-band surface pressure fit ABP) are stored in a separate Group ("Cloud") and information extracted and computed from ECMWF fields interpolated to the OCO-2 footprint are located in the Meteo group. Please note that the ECMWF data is based on the 3hourly forecast system and computation of added value products such as vapor pressure deficit has not been fully validated.

All important variables in the SIF-lite file should have corresponding attributes for units and standard names as well as a somewhat longer comment to describe the fields in more detail.

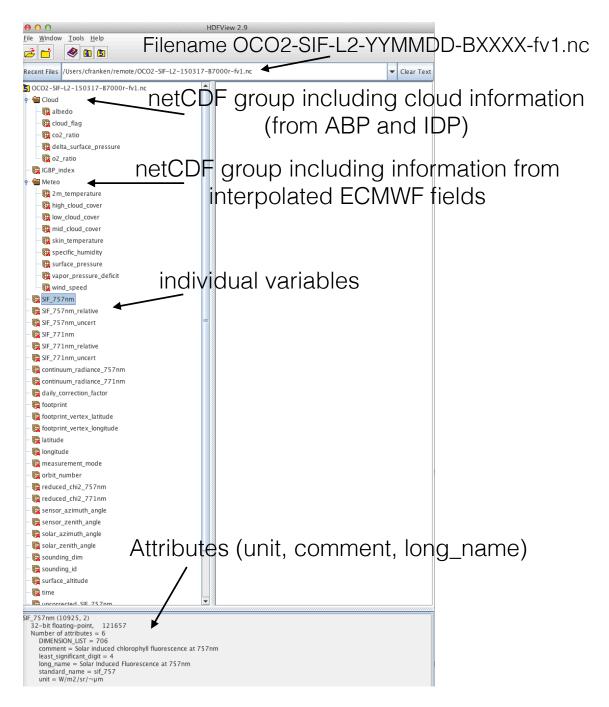


Figure 1: HDFview screenshot outlining the content of a SIF-lite file.

## File Structure & Fields

The primary variables that most users will need exist at the main level. In addition, there are some additional variables that certain users might want, contained in two groups within the file: Cloud and Meteo. Some NetCDF readers may not see these groups; if this happens, please update your NetCDF reader or use an HDF-5 reader.

#### Main level variables

Below, we will summarize all variables on the main level, starting with the most important variable first (those which initial users will focus on in the beginning).

KEY VARIABLES

latitude Latitude of the center of the OCO-2 footprint in the WGS 84 reference frame (degrees)

**longitude** Longitude of the center of the OCO-2 footprint in the WGS 84 reference frame. (degrees)

time time in seconds since 1993-01-01 00:00:00

SIF\_757nm Solar Induced Fluorescence at 757nm (W/m<sup>2</sup>/sr/ $\mu$ m)

SIF\_771nm Solar Induced Fluorescence at 771nm (W/m<sup>2</sup>/sr/ $\mu$ m). This value is typically about 1.5 times smaller than at 757nm and the two fields could be averaged after multiplication of sif\_771 with 1.5. However, we suggest to use them independently in the beginning as both may be affected by different bias sources and could provide robustness in the data analysis if both agree well.

SIF\_757nm\_uncert 1- $\sigma$  uncertainty in retrieved SIF at 757nm (W/m<sup>2</sup>/sr/ $\mu$ m)

SIF\_771nm\_uncert 1- $\sigma$  uncertainty in retrieved SIF at 771nm (W/m²/sr/ $\mu$ m). It is important to not that the  $1\sigma$  errors for both variables can be substantial. This can lead to negative SIF values, which are perfectly valid in a measurement retrieval sense owing to the presence of retrieval noise. Discarding negative values is dangerous as it biases the average. In general, multiple soundings will need to be averaged to reduce the noise by a factor of  $1/\sqrt{n}$ , with n being the number of averages.

Cloud/o2\_ratio Ratio of retrieved vs. predicted O<sub>2</sub> column using the 771nm retrieval window (used for initial cloud screening, ususally values >0.9 are sufficient for SIF related cloud screening as the ABP filters may be too strict). The most cloudy scenes are already pre-filtered in this dataset.

daily\_correction Daily Correction Factor Correction factor to estimate daily average SIF from instantaneous SIF (using pure geometric incoming light scaling). Especially at high latitudes, the fluorescence signal at 13:30 local solar overpass time cannot be directly compared with GPP since the length of day and variability of the solar zenith angle has to be taken into account. Under cloud-free conditions and ignoring Rayleigh scattering as well as gas absorption, the downwelling solar radiation scales linearly with  $\cos(SZA)$ . If  $t_0$  denotes the time of measurement in fractional days, a first order approximation for a daily fluorescence average can be written as:

$$\overline{F_S} = F_s / \cos(SZA(t_0)) \cdot \int_{t=t_0-12h}^{t=t_0+12h} \cos(SZA(t))dt$$

The aforementioned correction  $\cos(SZA(t_0)) \cdot \int_{t=t_0-12h}^{t=t_0+12h} \cos(SZA(t)) dt$  is saved in  $daily\_correction$ , computing the integral numerically in 10 minute time-steps (Using pyEphem (http://rhodesmill.org/pyephem/) to compute SZA as a function of latitude, longitude and time).

- IGBP index IGBP Index One-Minute Land Ecosystem Classification Product is a global (static map) data set of the International Geosphere-Biosphere Programme (IGBP) classification scheme stored on an equal-angle rectangular grid at 1-minute resolution. See http://modis-atmos.gsfc.nasa.gov/ECOSYSTEM/
- solar\_zenith\_angle Solar Zenith Angle (degrees): Solar zenith angle is the angle between the line of sight to the sun and the local vertical
- measurement\_mode OCO-2 Measurement mode, 0=Nadir, 1-Glint, 2=Target OCO-2 Measurement mode, 0=Nadir, 1-Glint, 2=Target, users should separate those for the analysis!

ADDITIONAL GEOMETRY/TIME VARIABLES

- sensor\_zenith\_angle Sensor Zenith Angle (degrees): Sensor zenith angle is the angle between the line of sight to the sensor and the local vertical
- sensor\_azimuth Sensor Azimuth Angle (degrees): Azimuth angle between line of sight and local north
- solar\_azimuth Solar Azimuth Angle (degrees): Azimuth angle between the solar direction as defined by the sounding location, and the sounding local north

time time in seconds since 1993-01-01 00:00:00

footprint\_id Detector Footprint Number: OCO-2 footprint identifier (1-8), identifying the 8 independent OCO-2 spatial samples per frame

sounding\_id Unique Indentifier for each sounding (YYYYMMDDHHMMSS)

altitude Surface Altitude Surface altitude of observed footprint (meters)

orbit\_number Orbit Number

footprint\_latitude\_vertices Latitude corner coordinates of the sounding location

footprint\_longitude\_vertices Longitude corner coordinates of the sounding location

#### OTHER VARIABLES

- uncorrected\_SIF\_771nm raw Solar Induced Fluorescence at 771nm (without any bias correction) (W/m<sup>2</sup>/sr/ $\mu$ m) Solar induced chlorophyll fluorescence at 771nm (without any bias correction)
- uncorrected\_SIF\_757nm raw Solar Induced Fluorescence at 757nm (without any bias correction) (W/m<sup>2</sup>/sr/ $\mu$ m) Solar induced chlorophyll fluorescence at 757nm (without any bias correction)
- uncorrected\_SIF\_771nm\_relative Solar Induced Fluorescence at 771nm in fractions of continuum level Solar induced chlorophyll fluorescence at 771nm in fractions of continuum level
- uncorrected\_SIF\_757nm\_relative Solar Induced Fluorescence at 757nm in fractions of continuum level, no bias correction Solar induced chlorophyll fluorescence at 757nm in fractions of continuum level, no bias correction
- continuum\_radiance\_757nm Continuum level radiance in the 757nm retrieval window  $(W/m^2/sr/\mu m)$
- continuum\_radiance\_771nm Continuum level radiance in the 771nm retrieval window  $(W/m^2/sr/\mu m)$ , note: this multiplies the OCO-2 radiance with a factor 2 to account for unpolarized light and units are converted as well.

reduced\_chi2\_757nm reduced  $\chi^2$  of the retrieval residuals in the 757nm window reduced\_chi2\_771m reduced  $\chi^2$  of the retrieval residuals in the 771nm window

#### Meteo group variables

**Specific\_humidity** Specific humdity at surface layer at the sounding location (ECMWF forecast)

vapor\_pressure\_deficit Vapor pressure deficit at the sounding location (2m) (ECMWF forecast, Pa)

skin\_temperature K Skin temperature at the sounding location (ECMWF forecast, K)

**2m\_temperature** 2m temperature at the sounding location (ECMWF forecast)

wind\_speed surface wind speed at sounding location (ECMWF forecast, m/s)

low\_cloud\_cover Cloud cover for low clouds (ECMWF forecast)

mid\_cloud\_cover Cloud cover for medium alt. cloud (ECMWF forecast)

high\_cloud\_cover Cloud cover for high clouds (ECMWF forecast)

surface\_pressure Surface pressure at the sounding location (ECMWF forecast, Pa)

#### Cloud group variables

- surface\_albedo\_760 Surface albedo (lambertian equivalent) as retrieved in the ABO2 preprocessor at 760nm
- cloud\_flag Cloud Flag from ABO2 (0-Classified clear, 1=Processing failed, 2=Not classified)
- delta\_pressure Retrieved-predicted surface pressure (Pa) from ABO2 (usable as cloud screener)
- co2\_ratio Ratio of CO<sub>2</sub> retrieved in weak and strong CO<sub>2</sub> band (value near 1 indicate scattering free scene)
- o2\_ratio Ratio of retrieved vs. predicted O<sub>2</sub> column using the 771nm retrieval window (used for initial cloud screening, ususally values >0.9 are sufficient for SIF related cloud screening as the ABP filters may be too strict). The most cloudy scenes are already pre-filtered in this dataset.

# Quality Filtering

The data has been pre-filtered using the following criteria:

**altitude** > 0 to exclude oceans

SIF between -5 and 50 W/m<sup>2</sup>/sr/ $\mu$ m to exclude obvious high and low fliers (rare)

 $\chi^2$  between 0 and 2 to exclude fits that don't represent the spectrum well

Continuum Level Radiance between 28 and 195 W/m<sup>2</sup>/sr/ $\mu$ m (too low and too bright scenes might be more affected by detector calibration)

**Solar Zenith Angle** <70 to remove retrievals with too high airmasses, for which rotational Raman scattering might be important

O2 ratio between 0.85 and 1.5 to exclude most cloudy scenes

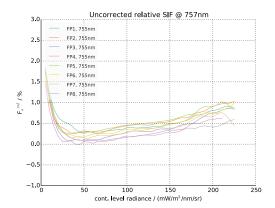
CO2 ratio between 0.5 and 4 to exclude most cloudy scenes

It has to be noted that this quality filtering is much relaxed compared to the OCO-2 XCO<sub>2</sub> lite file generation as SIF is less susceptible to atmospheric scattering. In addition, SIF retrievals are, as opposed to XCO<sub>2</sub>, accurate but imprecise, so that averaging of multiple data-points is required. Also not that clouds don't affect SIF signal strongly (Frankenberg et al, 2012).

#### Bias correction

The SIF retrievals presented here are based on the retrieval methodologies described in Frankenberg et al (2011a,b). The main retrieval quantity in the retrieval state vector is relative fluorescence, i.e. the fractional contribution of SIF to the continuum level radiance. Absolute SIF is being generated in the post-processing step. Owing to various effects such as uncertainties in the exact instrument line-shape per footprint or slight uncertainties in detector linearity, biases in retrieved SIF can occur. Here, we follow a similar strategy as in Frankenberg et al (2011b), using reference targets to correct for biases in SIF. Owing to the large amount of OCO-2 data, we can now perform these corrections on a daily basis. An example is shown in Figure 2.

There is room for improvement for this bias correction, specifically treating it separately for Glint and Nadir modes and using temporal smoothing of the correction curves. We appreciate any feedback as to the data quality and consistency to keep improving OCO-2 SIF-lite generation. The raw relative and absolute SIF values are provided in the datasets as well (see description above).



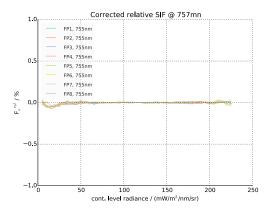


Figure 2: SIF-lite bias correction as a function of signal level (example taken from Oct. 2, 2014). Left: raw relative fluorescence retrievals over supposedly non-fluorescing surfaces. Right: Dataset after subtraction of the biases determined as a function of signal level

### References

- Frankenberg, C., Butz, A., & Toon, G. C. (2011a). Disentangling chlorophyll fluorescence from atmospheric scattering effects in O<sub>2</sub> A-band spectra of reflected sun-light. Geophysical Research Letters, 38, L03801.
- Frankenberg, C., Fisher, J., Worden, J., Badgley, G., Saatchi, S., Lee, J.-E., et al. (2011b). New global observations of the terrestrial carbon cycle from GOSAT: Patterns of plant fluorescence with gross primary productivity. Geophysical Research Letters, 38(17), L17706.
- Frankenberg, C., O'Dell, C., Berry, J., Guanter, L., Joiner, J., Khler, P., et al. (2014). Prospects for chlorophyll fluorescence remote sensing from the Orbiting Carbon Observatory-2. Remote Sensing of Environment, 147(0), 112.
- Guanter, L., Rossini, M., Colombo, R., Meroni, M., Frankenberg, C., Lee, J.-E., & Joiner, J. (2013). Using field spectroscopy to assess the potential of statistical approaches for the retrieval of sun-induced chlorophyll fluorescence from ground and space. Remote Sensing of Environment, 133(0), 5261.
- Guanter, L., Frankenberg, C., Dudhia, A., Lewis, P. E., Gmez-Dans, J., Kuze, A., et al. (2012). Retrieval and global assessment of terrestrial chlorophyll fluorescence from GOSAT space measurements. Remote Sensing of Environment, 121, 236251.
- Lee, J.-E., Frankenberg, C., van der Tol, C., Berry, J. A., Guanter, L., Boyce, C. K., et al. (2013). Forest productivity and water stress in Amazonia: observations

from GOSAT chlorophyll fluorescence. Proceedings of the Royal Society B: Biological Sciences, 280(1761).

• Frankenberg, C., O'Dell, C., Guanter, L., & McDuffie, J. (2012). Remote sensing of near-infrared chlorophyll fluorescence from space in scattering atmospheres: implications for its retrieval and interferences with atmospheric CO<sub>2</sub> retrievals. Atmospheric Measurement Techniques, 5(8), 20812094.